

Localized Edge Vibrations And Edge Reconstruction By Joule Heating In Graphene Nanoflakes

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ABSTRACT

Vibrations are often treated by very simple methods compared to electrons, but the precise atomic configuration becomes important for the stability of conductors when their size approaches nanometer scales. Graphene flakes are an example of a system, where atomically precise calculations are needed.

Control of the edge topology of graphene nanostructures is critical to graphene-based electronics. A means of producing atomically smooth zigzag edges using electronic current has recently been demonstrated in experiments [1]. We develop a microscopic theory for current-induced edge reconstruction using density functional theory. Our calculations[2] provide evidence for localized vibrations at edge-interfaces involving unpassivated armchair edges. We demonstrate that these vibrations couple to the current, estimate their excitation by Joule heating, and argue that they are the likely cause of the reconstructions observed in the experiments

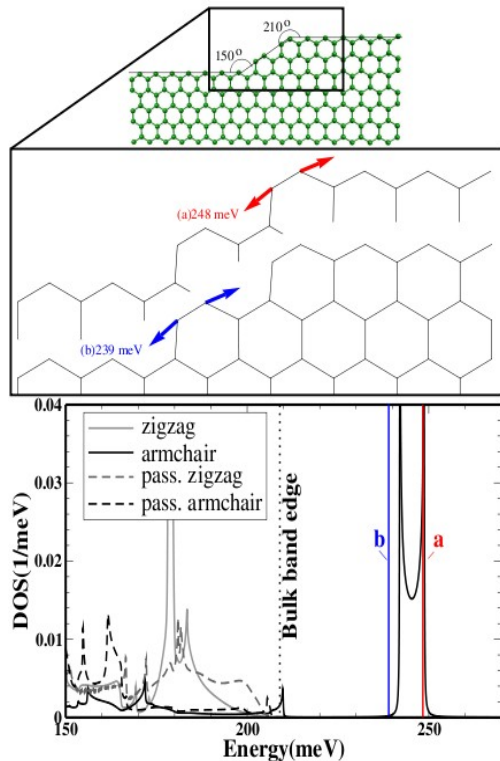


FIGURE 1. [Top] A graphene structure. [Middle] Two vibrational modes that accumulate energy at the edge. [Bottom] Vibrational density of states of the two modes compared to various edge structures.

REFERENCES

1. Jia *et al.*, *Science*, **323**, 1701, 2009.
2. Engelund *et al.*, *Physical Review Letters*, **104**, 036807, 2010.